

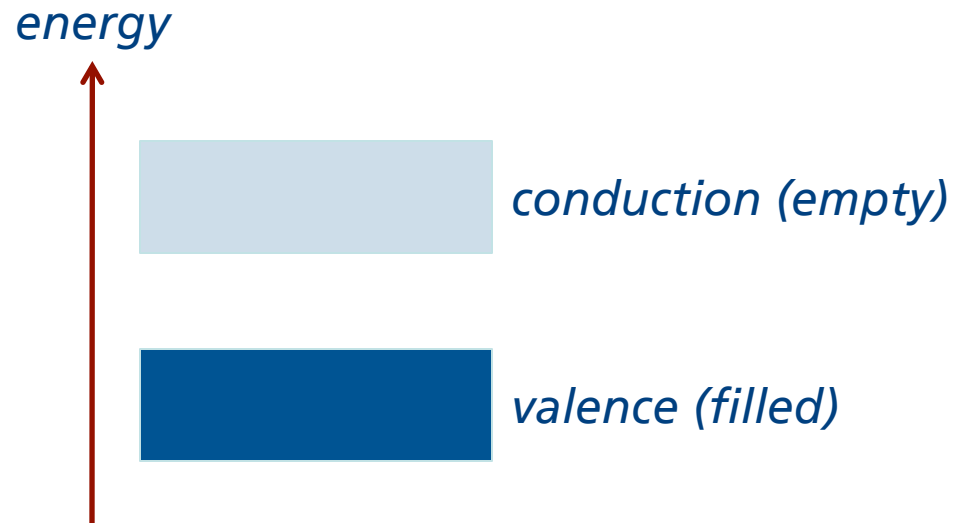
# 3D topological insulators and half-Heusler compounds

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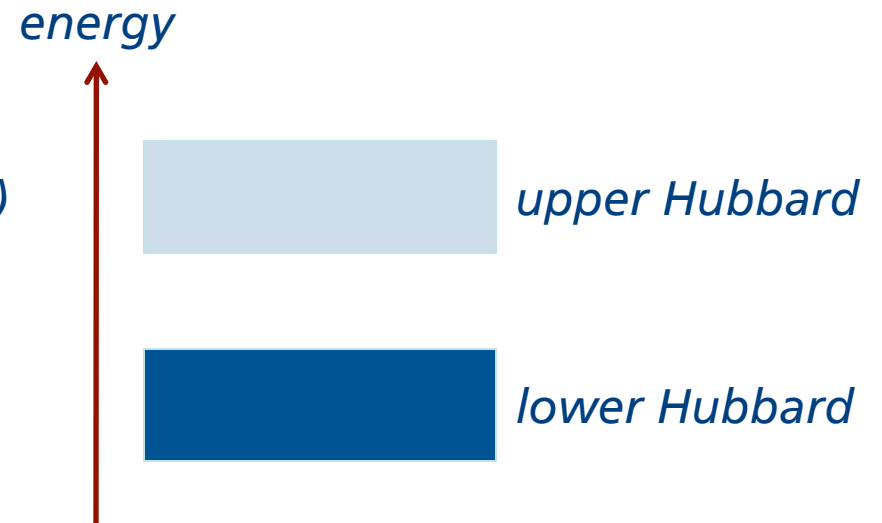
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## Trivial (normal) insulators:

### Band insulators: (eg. Si)

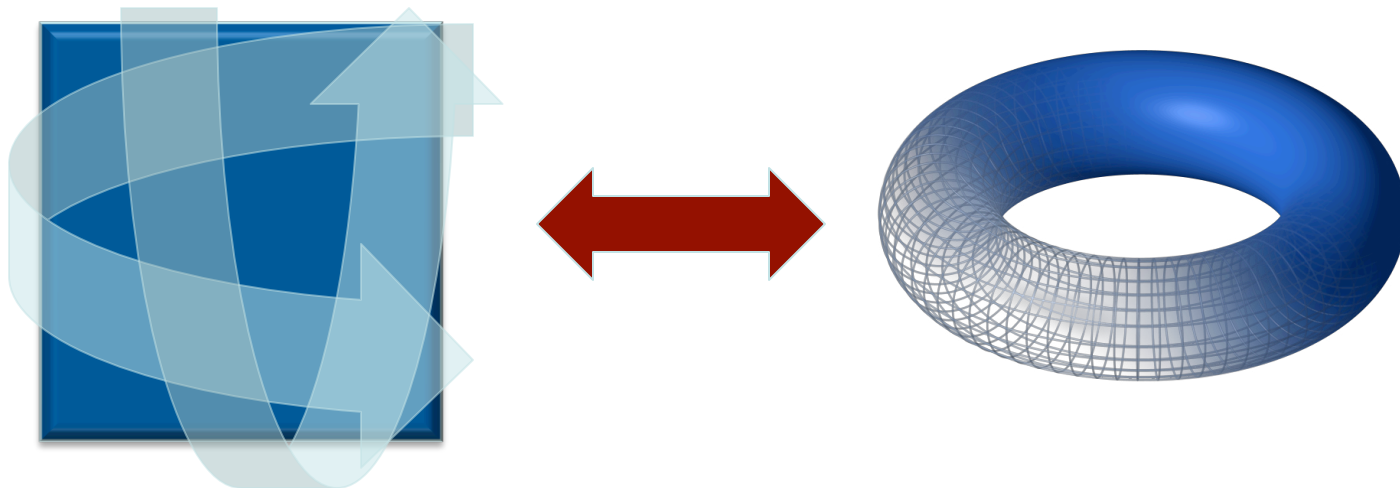


### Mott-Hubbard insulators: (eg. MnO)

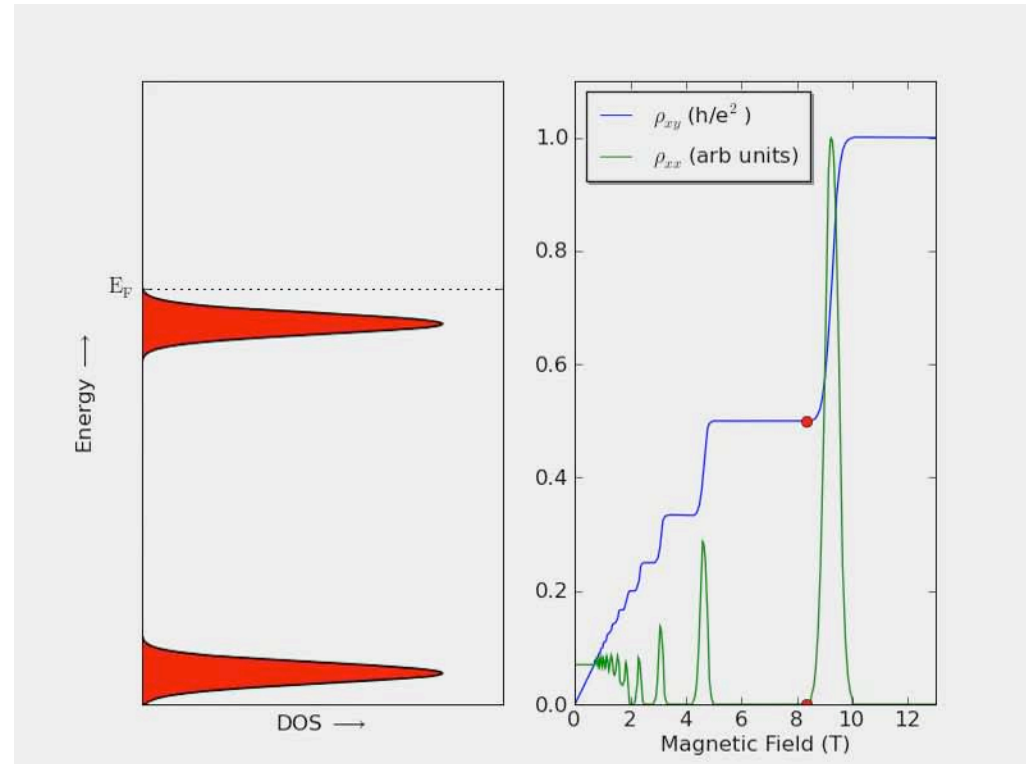
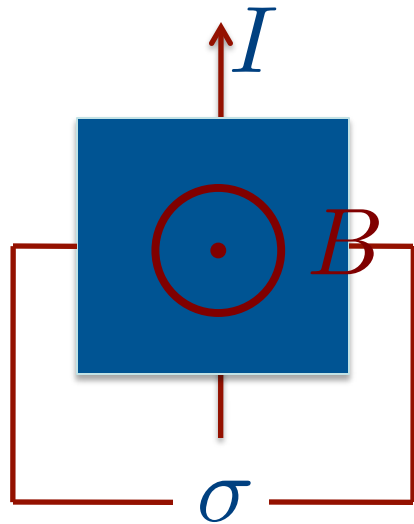


## Band structure and topology

*two-dimensional systems correspond to tori etc.*



## The quantum Hall effect:



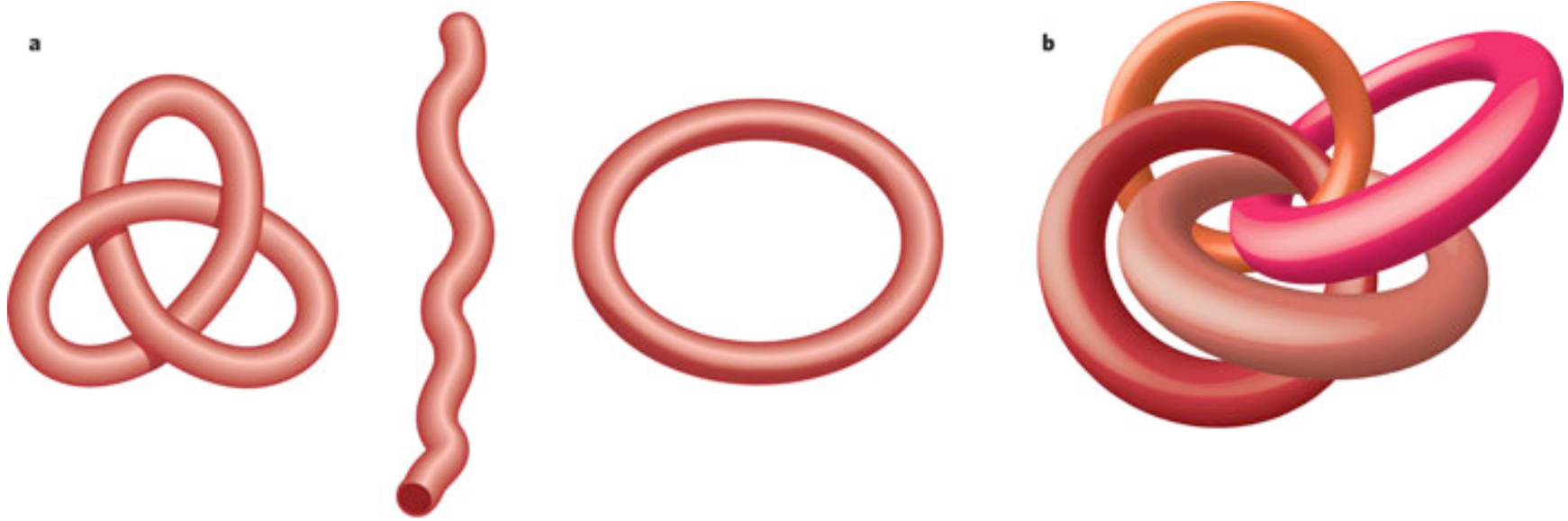
Landau levels of electrons in 2D orbiting an external magnetic field become highly degenerate at high fields. For sufficiently strong  $B$ -fields, each Landau level may have so many states that all of the free electrons in the system sit in only a few Landau levels and the quantum Hall effect is observed:

$$\sigma = \nu \frac{e^2}{h}$$

The suggestion by Haldane, Kane and others: [Moore, *Nature* 464 (2010) 194-197]

Instead of being driven by such an external magnetic field, electrons could, in principle, form a quantum Hall state driven by forces that result from spin-orbit coupling, a relativistic effect in which the spin and orbital angular momentum degrees of freedom of electrons are coupled; this coupling causes electrons that are moving through a crystal to feel a *spin-dependent* force, even in non-magnetic materials.

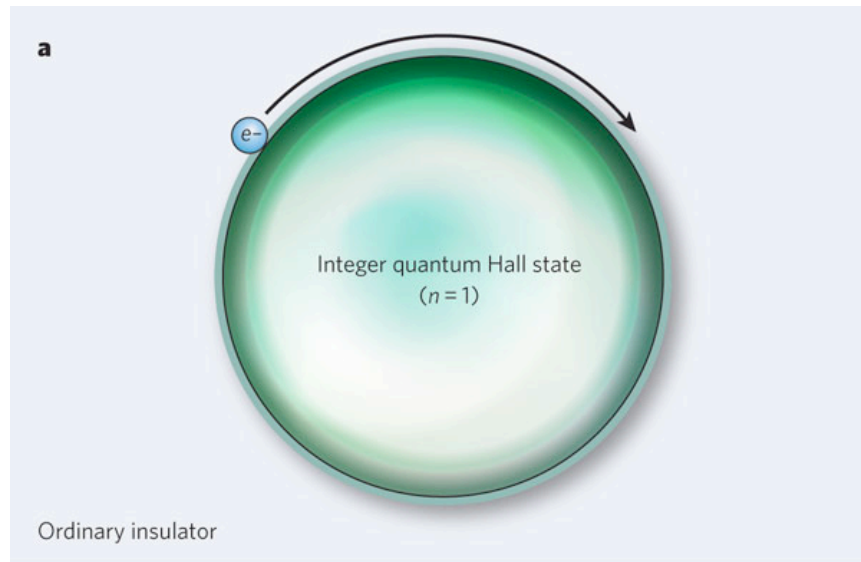
## The birth of topological insulators [Moore, *Nature* 464 (2010) 194-197]



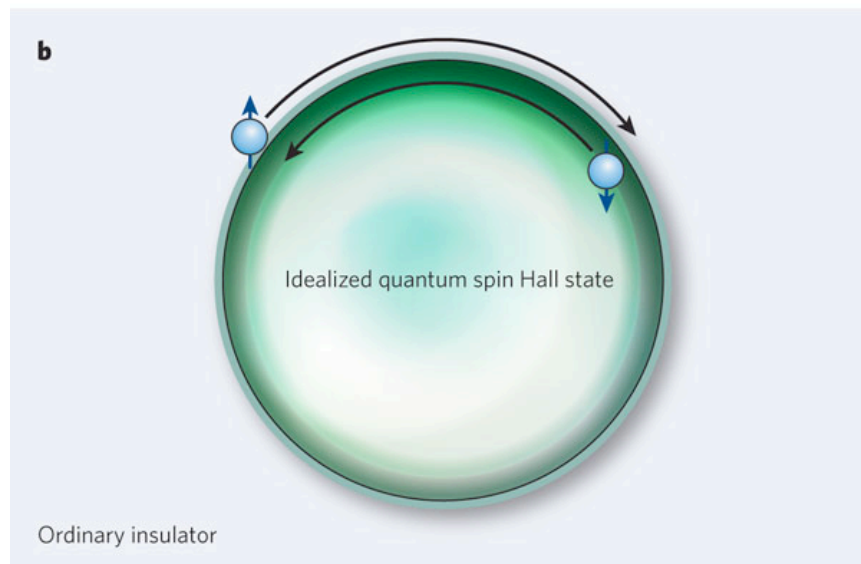
(a) An illustration of topological change and the resultant surface state. The trefoil knot (left) and the simple loop (right) represent different insulating materials: the knot is a topological insulator, and the loop is an ordinary insulator. Because there is no continuous deformation by which one can be converted into the other, there must be a surface where the string is cut, shown as a string with open ends (centre), to pass between the two knots; more formally, the topological invariants cannot remain defined. *If the topological invariants are always defined for an insulator, then the surface must be metallic.*

(b) The knotting in real topological insulators is more complex as these require a minimum of four electronic bands, but the surface structure that appears is relatively simple

## The birth of topological insulators [Moore, *Nature* 464 (2010) 194-197]

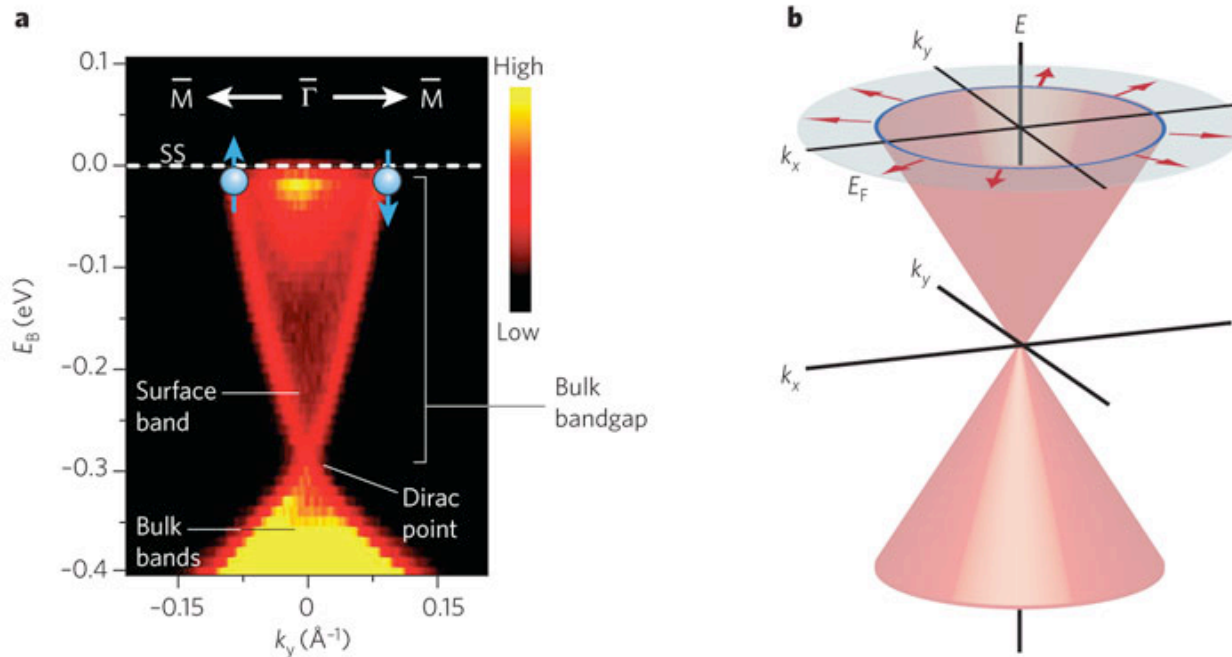


(a) Edge of an integer quantum Hall state. The electrons ( $e^-$ ) are confined to a 2D insulating droplet with a metallic edge. Along the edge, electrons propagate only in one direction, which is determined by the sign of the applied magnetic field perpendicular to the droplet.



(b) Edge of an idealized quantum spin Hall state (that is, a 2D topological insulator). Along the edge, spin-up electrons move clockwise, whereas spin-down electrons move anticlockwise. Spin-up and spin-down electrons are independent and are in oppositely directed quantum Hall states.

# The birth of topological insulators [Moore, *Nature* 464 (2010) 194-197]

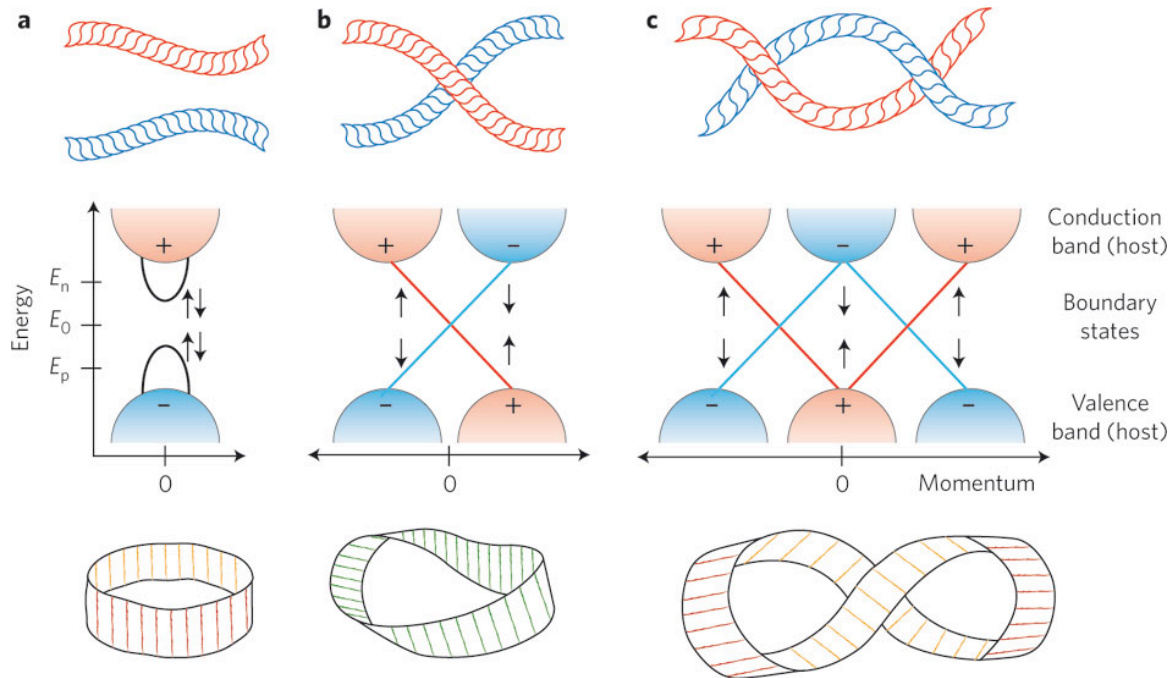


(a) The electronic structure of  $\text{Bi}_2\text{Se}_3$ , as measured by ARPES. Measured energy electron energy,  $E_B$ , is plotted against electron momentum,  $k_y$ . High intensity (red and yellow areas) indicates a non-zero electronic density of states. The surface bands crossing the bulk bandgap enclose a single Dirac point at the Brillouin-zone centre ( $\Gamma$ ), which is the signature that this material is a topological insulator. indicates the centre of an edge of the Brillouin zone, and the path in the Brillouin zone is indicated by white arrows. The direction of electron spin is indicated by blue arrows.

(b) Theoretical idealization of the electronic structure of  $\text{Bi}_2\text{Se}_3$ , showing the rotation of the spin degree of freedom (red arrows) as an electron (with energy  $E$ ) moves around the Fermi surface (with Fermi energy  $E_F$ ).



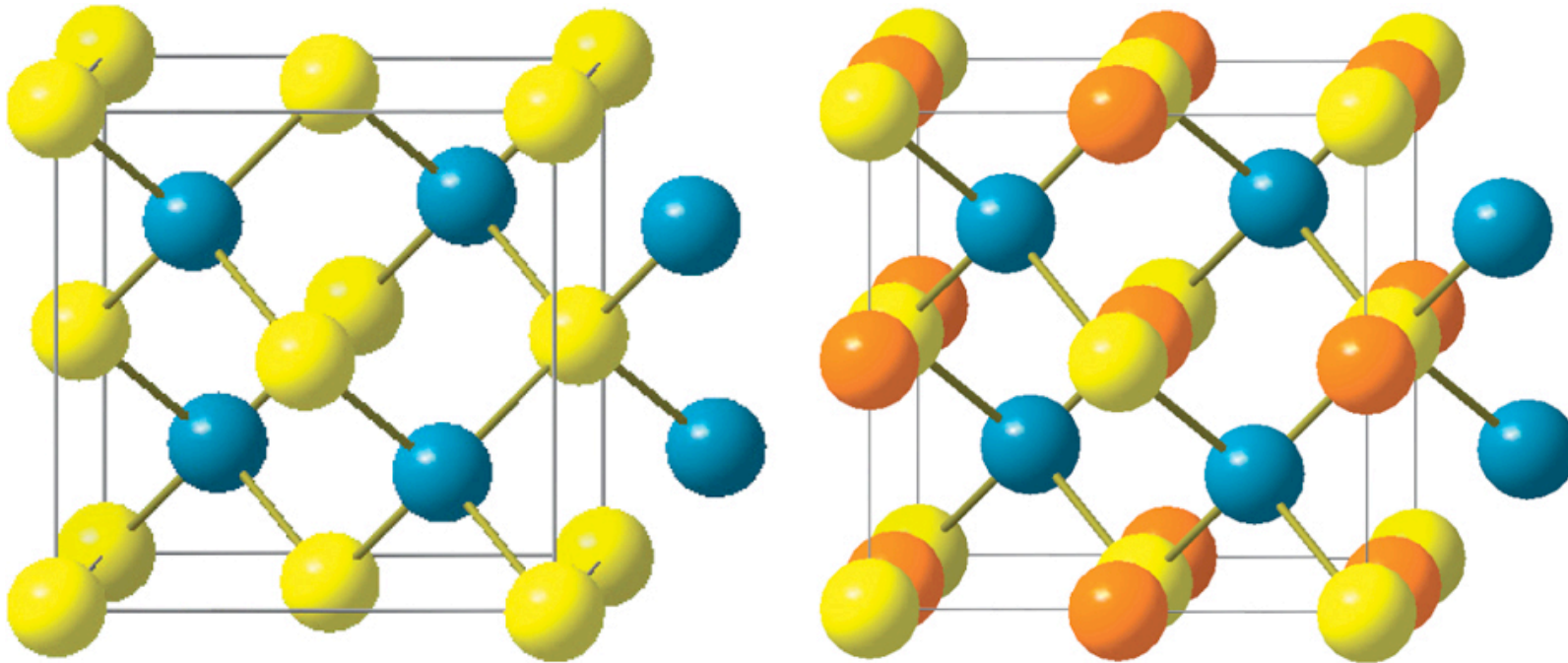
# Topological insulators, A romance with many dimensions [Manoharan, *Nature Nanotechnol.* 5 (2010) 477-479]



(a) The conduction and valence bands of a typical 3D solid (middle section). The shaded regions are the bands in the bulk of the solid, and the thick black lines are the bands at the surface. In general, the conduction band is symmetric (red), the valence band is antisymmetric (blue), and spin-up and spin-down electrons (black arrows) have the same energy. (b) Spin-orbit coupling lifts the degeneracy of the electron spins and leads to other changes: in the bulk, for example, the conduction band becomes antisymmetric (-) and the valence band becomes symmetric (+). At the boundary the bands (the red and blue lines) actually cross over each other, and the Fermi energy is forced to intersect both bands, which results in the conduction of electric charge along the boundary.

# Tunable multifunctional topological insulators in ternary Heusler compounds

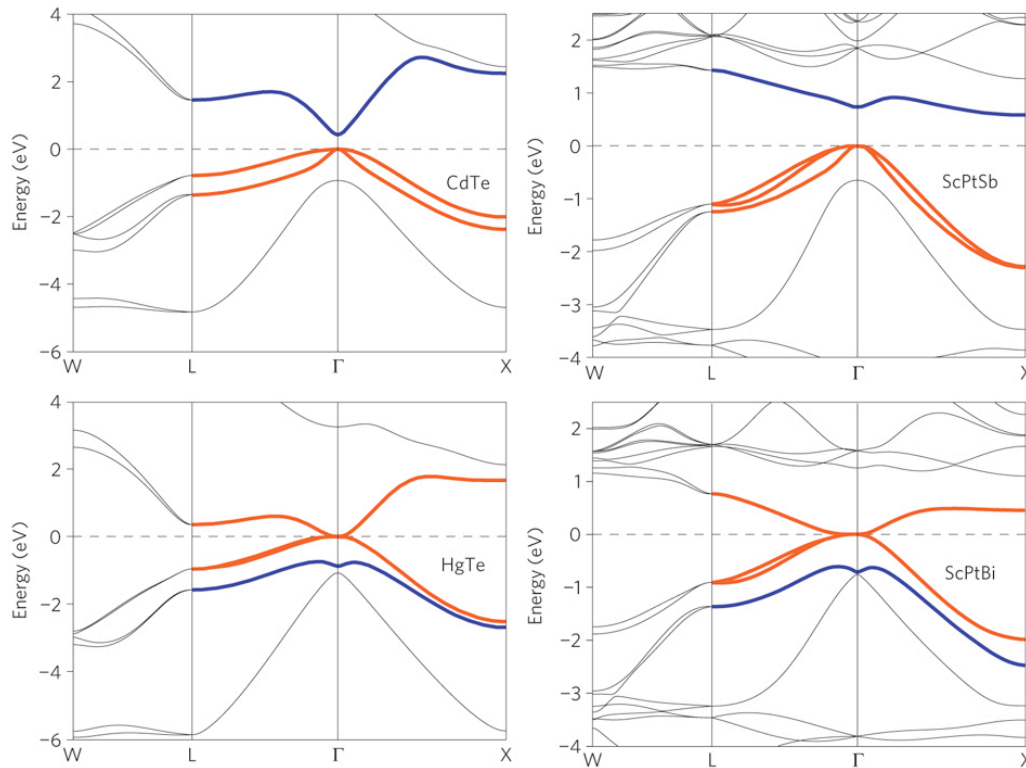
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The zinc-blende (XY) structure is shown on the left, and the C1b (XYZ) on the right. Yellow and blue spheres correspond to the main-group (Z) and transition (Y) elements, respectively. The orange spheres in C1b stand for the additional stuffing (X) element.

# Tunable multifunctional topological insulators in ternary Heusler compounds

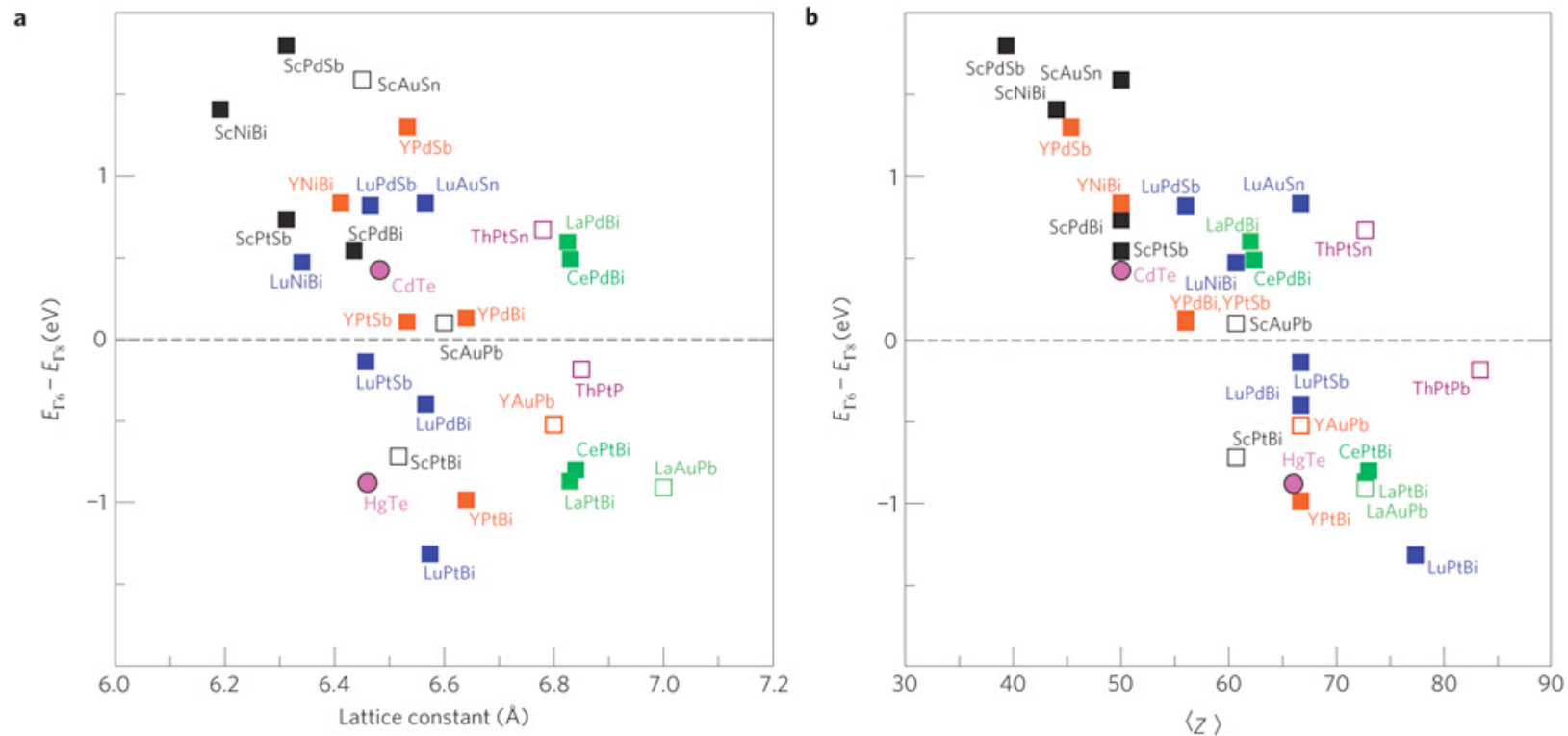
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Red colour marks the bands with  $\Gamma_8$  symmetry, blue with  $\Gamma_6$ . Comparison reveals obvious similarity between binary systems and their ternary equivalents: both CdTe and ScPtSb are trivial semiconductors with  $\Gamma_6$  situated above  $\Gamma_8$ , which sits at the Fermi energy (set to zero). Both HgTe and ScPtBi are topological with inverted band order; the band with  $\Gamma_6$  symmetry is situated below  $\Gamma_8$ .

# Tunable multifunctional topological insulators in ternary Heusler compounds

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HgTe and CdTe binaries are shown for comparison. Open squares mark the systems not reported in the literature. (a)  $E_{\Gamma_6} - E_{\Gamma_8}$  difference as a function of the lattice constant. The borderline compounds (between trivial and topological) insulators (YPtSb, YPdBi, ScAuPb) are situated closer to the zero horizontal line. (b)  $E_{\Gamma_6} - E_{\Gamma_8}$  difference as a function of the average spin-orbit coupling strength represented by the average nuclear charge per formula.